Two-loop self-energy correction to the ground-state Lamb shift in H-like ions

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Abstract

The two-loop self-energy correction is evaluated to all orders in $Z\alpha$ for the ground-state Lamb shift of H-like ions with $Z \geq 20$, where Z is the nuclear charge number and α is the fine structure constant. The results obtained are compared with analytical calculations performed within the $Z\alpha$-expansion.

Key words: self-energy, Lamb shift, QED corrections
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The subject of this paper is a study of the historically most problematic two-loop QED effect for the Lamb shift of H-like ions, the two-loop self-energy correction. Traditionally, investigations of radiative corrections to a given order in the fine-structure constant α rely on an expansion in the parameters $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$ (Z is the nuclear charge number). For the two-loop self-energy correction, the energy shift is conveniently expressed in terms of a dimensionless function $F(Z\alpha)$,

$$\Delta E = m \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} F(Z\alpha)\,, \tag{1}$$

which expansion reads

$$F(Z\alpha) = B_{40} + (Z\alpha) B_{50} + (Z\alpha)^2 \Big[L^3 B_{63} + L^2 B_{62} + L\, B_{61} + G_{\rm h.o.}(Z\alpha)\Big]\,,$$

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(2)

where $L = \ln[(Z\alpha)^{-2}]$, n is the principal quantum number, and the remainder $G_{\rm h.o.}(Z\alpha)$ incorporates all higher-order terms. Calculations of the coefficients of this expansion extended over several decades [1,2,3,4,5,6],

$$B_{40}(ns) = 1.409\,244\ldots\,, \tag{3}$$
$$B_{50}(ns) = -24.2668(31)\,, \tag{4}$$
$$B_{63}(ns) = -8/27\,, \tag{5}$$
$$B_{62}(1s) = 16/27 - (16/9)\ln 2\,, \tag{6}$$
$$B_{61}(1s) = 49.838317\,. \tag{7}$$

The expansion of the higher-order remainder $G_{\rm h.o.}$ starts with a constant, $G_{\rm h.o.}(Z\alpha) = B_{60} + Z\alpha(\cdots)$. A partial result for the B_{60} coefficient was obtained recently by Pachucki and Jentschura [7],

$$B_{60} = -61.6(3) \pm 15\%\,, \tag{8}$$

where $\pm 15\%$ refer to the possible contribution of uncalculated terms. One of the notable features of the expansion (2) is its remarkably slow convergence, even for low values of the nuclear charge number Z, which exhibits itself by large numerical values of the expansion coefficients B_{ij}. This makes clear that a direct evaluation of the two-loop self-energy correction is highly desirable, especially when addressing middle- and high-Z ions.

Calculations of the two-loop self-energy correction (Fig. 1) to all orders in the parameter $Z\alpha$ started with the irreducible contribution of the diagram (a) (also known as the *loop-after-loop* (LAL) correction), which is by far the simplest part of the total set. Such evaluation was first accomplished by Mitrushenkov *et al.* [8] and later by other authors [9,10]. The contribution of the remaining diagrams in Fig. 1 is by far more difficult to calculate. First attempt to evaluate it to all orders in $Z\alpha$ was made by Mallampalli and Sapirstein [11]. In that work, the contribution of interest was rearranged in 3 parts, referred to by the authors as the "M", "P", and "F" terms. Mallampalli and Sapirstein calculated only the M and F terms, while the P term was left out since a new numerical technique had to be developed for its computation. In addition, since the numerical procedure turned out to be very time consuming, the actual calculation of the M term was carried out only for two ions, uranium and bismuth. Subsequently, in the investigation by two of us [12], a computation of the remaining P term for $Z = 83$, 90, and 92 was performed, which formally accomplished the calculation of the two-loop self-energy for these ions.

First complete evaluation of all contributions to the two-loop self-energy cor-

rection to all orders in $Z\alpha$ was carried out in our recent investigations [13,14] for the ground-state Lamb shift of H-like ions with $Z \geq 40$. In the present work, we extend our calculation to the ions with $Z = 20$, 30 and improve the accuracy of the previous numerical results for $Z = 40$-60.

It is beyond the scope of the present paper to describe all modifications of the numerical procedure that allowed us to obtain improved numerical results in the low-Z region, despite the occurrence of large numerical cancellations that tend to grow very fast as Z decreases. We only mention that the new *dual-kinetic-balance* basis set [15] constructed with B splines was employed in our calculations of the P term, which considerably improved the convergence with respect to the number of basis functions in the low-Z region. Another problem that was encountered in the evaluation of the P term was to keep numerical integrations over momentum variables well under control. This problem is associated with a significant contribution coming from the region of very large momenta, where the numerical Green function is not smooth enough, due to restrictions of a finite-basis-set representation. The problem was solved by introducing a set of subtractions that have the same behaviour for large momenta as the original integrand but are easier to evaluate numerically, and by employing very fine grids for numerical momentum integrations. The calculation of the M term was carried out employing the contour C_{LH} for the integrations over the virtual photon energies (see Ref. [14]) that is much more suitable for the numerical evaluation in the low-Z region than the integration simply along the imaginary axis. In addition, it turned out to be possible to separate from the M term a contribution, which contains the dominant part of the spurious terms in the low-Z region that are cancelled in the final sum, and to calculate it separately. This contribution contains only one free partial-wave expansion parameter, which makes the corresponding numerical computation much easier as compared to the full M term that has a partial-wave expansion over two independent parameters.

Numerical results obtained for the two-loop self-energy correction for the ground state of H-like ions are presented in Table 1 in terms of the function $F(Z\alpha)$ defined by Eq. (1). As compared to our previous investigations [13,14], we performed calculations for $Z = 20$, 30 and improved the numerical accuracy of the results for the P and M terms for $Z = 40$, 50, and 60. The values for $Z \geq 70$ are identical to those in our previous evaluation [14].

In Fig. 2 we compare our non-perturbative (in $Z\alpha$) results with contributions of the known coefficients of the expansion (2). The solid line corresponds to the first two terms in Eq. (2), whereas the dashed line represents a contribution of all known terms of the $Z\alpha$ expansion (including the result of Ref. [7] for B_{60}). In order to provide a more detailed comparison with the analytical results, we first separate the contribution containing all orders in $Z\alpha$ starting from

$(Z\alpha)^2$, defined as

$$\widetilde{F}(Z\alpha) = \frac{F(Z\alpha) - B_{40}}{Z\alpha} = B_{50} + (Z\alpha)(\cdots)\,. \tag{9}$$

The function $\widetilde{F}(Z\alpha)$ is plotted in Fig. 3. The cross on the picture represents its analytical value at $Z = 0$, B_{50}. It is noteworth that, despite the numerically large contributions B_{63}-B_{60} in the next-to-leading order, the behaviour of the function $\widetilde{F}(Z\alpha)$ is very smooth and that it tends to the analytical value at $Z = 0$.

Next, we separate the higher-order remainder $G^{\rm h.o.}(Z\alpha)$ [defined by Eq. (2)] from our non-perturbative results, with the corresponding plot presented in Fig. 4. The cross with the error bars corresponds to the analytical result of Ref. [7] for the B_{60} coefficient, $B_{60} = -62 \pm 9$. We see that the apparent limit of the numerical values at $Z \to 0$ seems to be about twice as large as the analytical result of Ref. [7]. However, we can not at present conclude whether this disagreement stems from the coefficient B_{60} or from one of the logarithmic coefficients in the order $\alpha^2(Z\alpha)^6$. A detailed comparison with individual coefficients can be in principle performed by fitting numerical results to the analytical form of the $Z\alpha$ expansion, but it requires an improvement of the accuracy of the numerical data. We mention also that a reliable extrapolation of the numerical data to $Z = 0$ is complicated by the presence of nearly-singular terms like $Z\alpha \ln Z\alpha$, $Z\alpha \ln^2 Z\alpha$ in the $Z\alpha$ expansion of the remainder $G^{\rm h.o.}$, which could possibly result in a rapidly-varying structure of $G^{\rm h.o.}(Z)$ near the origin. We hope that an extension of our calculations to lower values of Z and an improvement of numerical accuracy of the results will allow us to provide a more detailed comparison with analytical calculations.

In summary, we have performed calculations of the two-loop self-energy correction that extend our previous evaluations to the region $Z \geq 20$. The numerical results obtained are compared with the known terms of the $Z\alpha$ expansion. A good agreement is demonstrated with the first terms of this expansion. However, the numerical results are shown to be likely in a disagreement with the analytical results to order $\alpha^2(Z\alpha)^6$.

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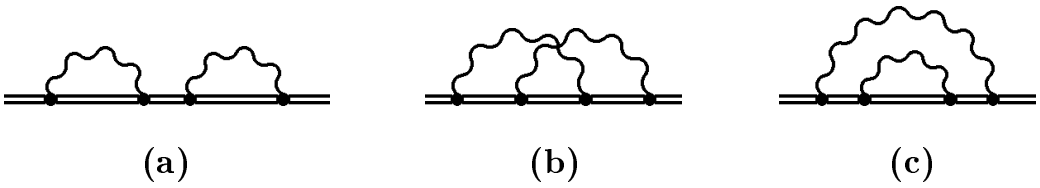

Fig. 1. Two-loop self-energy diagrams.

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Table 1
Individual contributions to the two-loop self-energy correction expressed in terms of $F(Z\alpha)$.

Z	LAL	F term	P term	M term	Total
20	−0.602	136.89(3)	−102.03(9)	−34.77(9)	−0.52(13)
30	−0.757	44.723(5)	−29.42(4)	−15.46(4)	−0.91(6)
40	−0.871	19.504(2)	−11.58(2)	−8.26(7)	−1.21(7)
			−11.41(15)[a]	−8.27(18)[a]	−1.05(23)[a]
50	−0.973	10.025(2)	−5.486(20)	−5.00(5)	−1.43(5)
			−5.41(8)[a]	−4.99(6)[a]	−1.34(10)[a]
60	−1.082	5.723(1)	−2.961(20)	−3.342(9)	−1.66(2)
			−2.93(4)[a]	−3.342(21)[a]	−1.63(4)[a]
70	−1.216	3.497	−1.757(25)	−2.412(11)	−1.888(27)
83	−1.466	1.938	−1.057(13)	−1.764(4)	−2.349(14)
92	−1.734	1.276	−0.812(10)	−1.513(3)	−2.783(10)
100	−2.099	0.825	−0.723(7)	−1.384(3)	−3.381(8)

[a] Ref. [14].

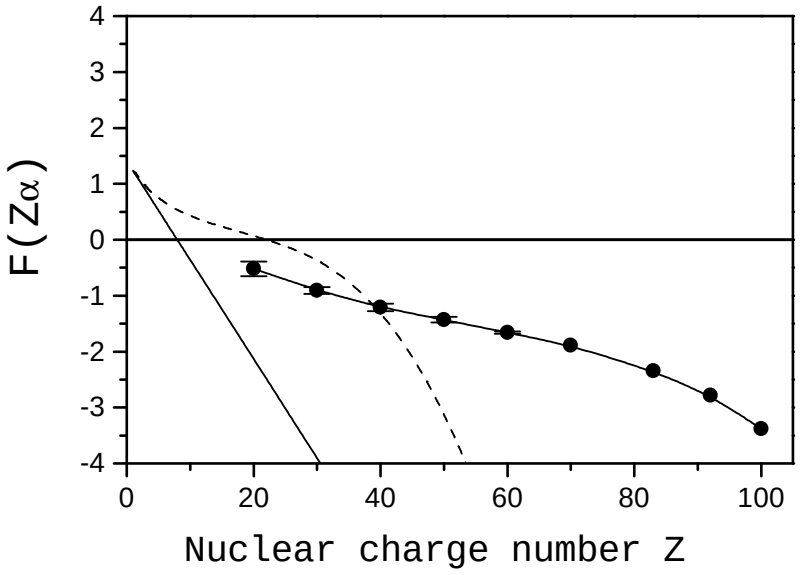

Fig. 2. The two-loop self-energy correction to all orders in $Z\alpha$ (dots) together with the contribution of the first two terms of the $Z\alpha$ expansion (2) (solid line) and all known terms of the $Z\alpha$ expansion (dashed line).

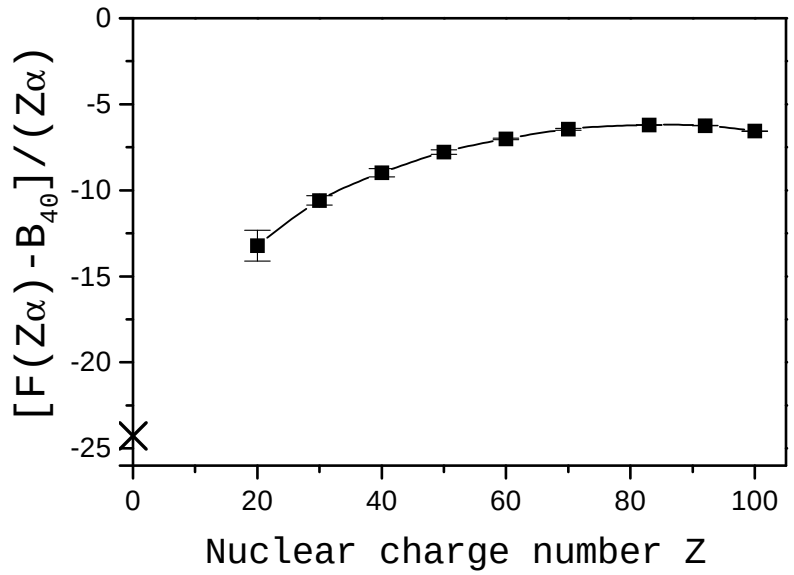

Fig. 3. Numerical results for the two-loop self-energy correction with the leading contribution of the $Z\alpha$ expansion subtracted out, as given by Eq. (9). The cross denotes the analytical value for this contribution at $Z = 0$ (i.e., the coefficient B_{50}).

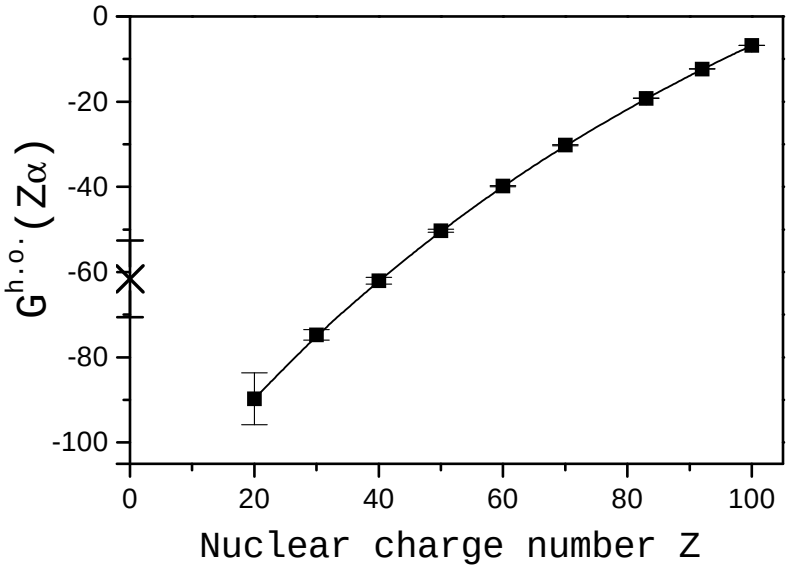

Fig. 4. Higher-order remainder $G^{\mathrm{h.o.}}(Z\alpha)$ defined by Eq. (2). The cross denotes the analytical result for this contribution at $Z = 0$ (i.e., the coefficient B_{60}) obtained in Ref. [7].